

# 20CY108 SPECTROSCOPIC METHODS FOR CHEMICAL ANALYSIS

Hours Per Week :

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3	1	-	4

## Course Description and Objectives:

This course will be providing students with understanding the basic knowledge including the working principles and applications of various instrumentation techniques to analyze the chemical substances both qualitative and quantitative approach. This course will cover the basic fundamental and working of various spectroscopic techniques including UV-visible, FT-IR, Raman, NMR, ESR, and MASS, as these spectroscopic techniques are very important role in the various industries. Throughout the course, students will learn analytical instrumentation techniques and the data interpretation used to elucidate the structure confirmation of chemical molecules.

## Course Outcomes:

Upon completion of the course, the student will be able to achieve the following outcomes:

COs	Course Outcomes
1.	Apply the basic concepts of absorption spectroscopic methods
2.	Determine the structures of organic compounds using NMR spectroscopic techniques.
3.	Evaluate the importance of advance NMR spectroscopic to interpret the structures of various organic compounds.
4.	Apply the basic knowledge of ESR spectroscopy to identify the ESR-active species.
5.	Analyze the structures of various organic compounds using mass spectrometric techniques.1

**Unit - I :****Absorption spectroscopy :**

Colorimetry, theory of colorimetry, derivation of Beer-Lambert's law, UV-Visible Spectroscopy: electronic transition, deviations from Beers law, solvent effect, Woodward-Fischer rule, calculation of  $\lambda_{\max}$  using Woodward-Fischer rule, single and double beam UV-visible spectroscopy - instrumentation with components, qualitative and quantitative applications. Fluorescence basic concept and applications. Infrared spectroscopy: molecular vibrations, degree of freedom, factors influencing vibrational frequencies, instrumentation, characteristic frequencies of organic molecules, qualitative and quantitative analysis. Raman spectroscopy: Raman effect and spectra, differences between Raman spectra and IR spectra, instrumentation

**Unit - II :**

**NMR Spectroscopy:** Introduction to NMR spectra, chemical shift, factors affecting chemical shift, shielding, spin-spin splitting, mechanism for spin-spin coupling, instrumentation, interpretation of NMR spectra of typical organic compounds.

**Unit - III :**

**Advanced NMR spectroscopy :** Factors influencing NMR spectra, Decoupling, DEPT, relaxation measurements (T1 and T2). FT-NMR, study of isotopes other than proton-<sup>13</sup>C, <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P, and <sup>11</sup>B. 2D NMR techniques: homo- and heteronuclear correlation (COSY, and NOESY).

**Unit - IV :**

**ESR Spectroscopy:** Principle, g value, hyper fine splitting, qualitative analysis, Kramers degeneracy, fine splitting, instrumentation, introduction to double resonance technique, difference between ESR and NMR, quantitative analysis, application to study of free radicals and other analytical applications.

**Unit - V :**

**Mass Spectrometry :** Principle, basic instrumentation, energetics of ion formation, types of peaks observed, resolution, qualitative analysis, molecular weight determination, quantitative analysis, and advantages, and MALDI-TOF.

**Text Books**

1. Instrumental methods of analysis – H.H Willard, Meritt Jr. and J.A Dean
2. Principles of instrumental analysis – Skoog and West
3. Vogels Textbook of Quantitative Inorganic analysis – J. Basset, R.C Denney, G.H Jefferey and J.Madhan
4. Instrumental methods of analysis – B.K Sarma, Goel Publishing House, Meerut
5. Instrumental methods of Analysis – Chatwal and Anand
6. Instrumental methods of Analysis – Ewing

**Reference Books:**

1. Instrumental methods of Analysis – Galen S. Ewing, Mcgraw Hill Higher Education, 5 th edition, 1985
2. Handbook of Instrumental techniques for Analytical Chemistry, Frank Settle, Prentice Hall, 1997.
3. Analytical Chemistry – J.G. Dick, McGraw Hill Publishers, 1975.
4. R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, (1986) Addison Wesley, Longman Ltd, London.
5. Analytical Chemistry Principles – J.H. Kennedy, Saunders College Publishing, New York, II Edition, 1990.
6. Instrumental Methods of Chemical Analysis – G.W. Ewing, McGraw Hill Publishers, 1975.